



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:32 pm BST

PDB ID : 1GGU  
Title : HUMAN FACTOR XIII WITH CALCIUM BOUND IN THE ION SITE  
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Deposited on : 1998-07-22  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

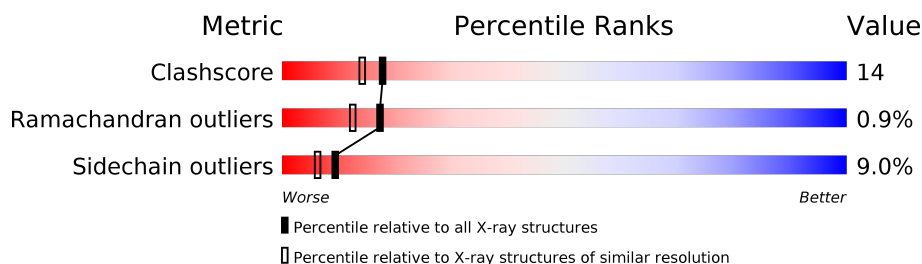
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	
1	B	731	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12297 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5627	3571	967	1063	26			
1	B	707	Total	C	N	O	S	0	0	0
			5667	3595	975	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	GLU	GLN	CONFLICT	UNP P00488
B	567	GLU	GLN	CONFLICT	UNP P00488

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

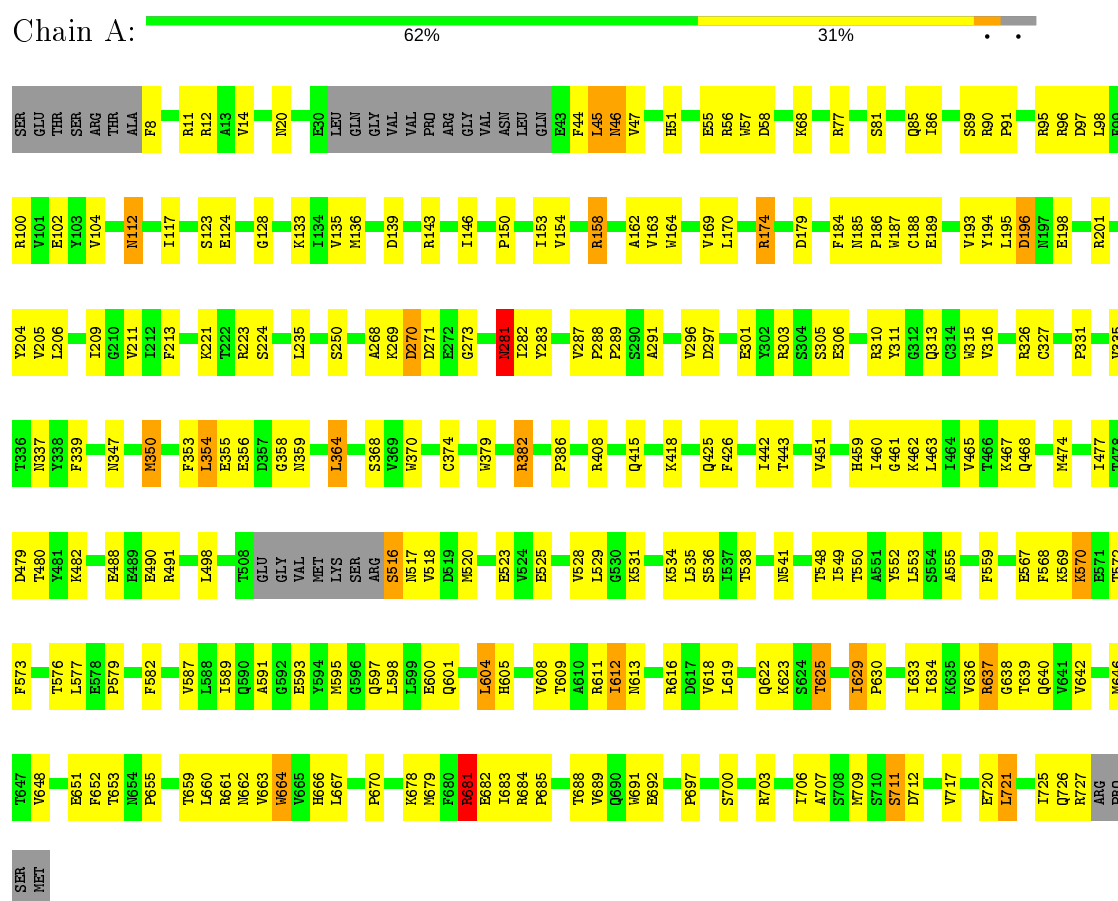
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total	O	0	0
			437	437		
3	B	564	Total	O	0	0
			564	564		

### 3 Residue-property plots

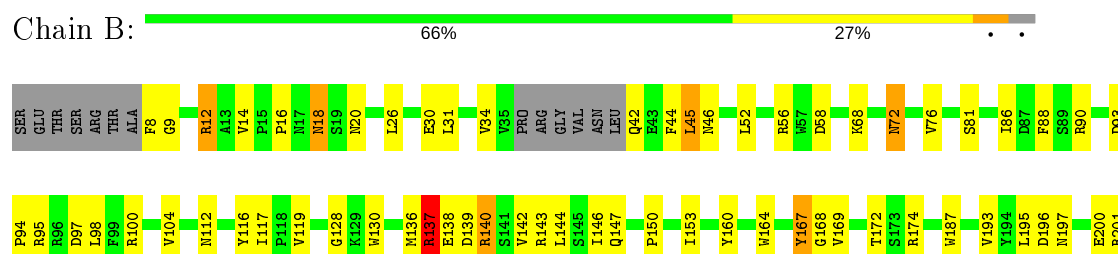
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: PROTEIN (COAGULATION FACTOR XIII)



#### • Molecule 1: PROTEIN (COAGULATION FACTOR XIII)





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.17Å 70.76Å 133.82Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.9 (20.00-2.10)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.227 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.79	1/5760 (0.0%)	0.95	8/7817 (0.1%)
1	B	0.83	0/5800	0.96	9/7871 (0.1%)
All	All	0.81	1/11560 (0.0%)	0.96	17/15688 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	664	TRP	CB-CG	-5.13	1.41	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	LEU	N-CA-C	-7.13	91.74	111.00
1	B	9	GLY	N-CA-C	-7.06	95.45	113.10
1	A	174	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	158	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	158	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	174	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	382	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	196	ASP	N-CA-C	5.67	126.30	111.00
1	B	58	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	137	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	588	LEU	CA-CB-CG	5.46	127.85	115.30
1	B	382	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	382	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	56	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	408	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	86	ILE	CB-CA-C	-5.13	101.34	111.60
1	A	11	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5627	0	5478	166	0
1	B	5667	0	5512	147	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	437	0	0	14	0
3	B	564	0	0	14	0
All	All	12297	0	10990	304	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PRO:HG2	1:A:379:TRP:HB3	1.26	1.13
1:A:633:ILE:HB	1:A:651:GLU:HB3	1.51	0.89
1:B:44:PHE:O	1:B:45:LEU:HB2	1.74	0.86
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.59	0.83
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.44	0.82
1:B:31:LEU:HD22	1:B:167:TYR:O	1.82	0.79
1:A:443:THR:HB	1:A:451:VAL:HG13	1.64	0.78
1:A:567:GLU:HG2	1:A:570:LYS:HD2	1.64	0.76
1:A:354:LEU:HD23	1:A:618:VAL:HG11	1.68	0.76
1:A:518:VAL:HG12	1:A:619:LEU:HD11	1.69	0.74
1:A:44:PHE:O	1:A:45:LEU:HB2	1.86	0.73
1:B:674:ARG:HD2	1:B:675:PRO:HD2	1.71	0.73
1:A:612:ILE:HG22	1:A:613:ASN:H	1.53	0.73
1:A:136:MET:HB3	1:A:143:ARG:HB3	1.70	0.72
1:B:604:LEU:HB2	1:B:625:THR:HG22	1.69	0.72
1:A:605:HIS:CE1	1:A:622:GLN:HE21	2.08	0.71
1:B:12:ARG:HD3	3:B:6149:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:ND2	1:A:188:CYS:HB2	2.06	0.70
1:B:548:THR:HG22	1:B:613:ASN:ND2	2.07	0.70
1:B:548:THR:HG22	1:B:613:ASN:HD22	1.59	0.68
1:A:46:ASN:OD1	1:A:89:SER:HB3	1.95	0.67
1:A:666:HIS:O	1:A:707:ALA:HA	1.94	0.67
1:A:660:LEU:O	1:A:682:GLU:HA	1.95	0.67
1:A:549:ILE:HG22	1:A:550:THR:N	2.11	0.65
1:B:704:LYS:HD2	1:B:720:GLU:OE1	1.96	0.65
1:A:211:VAL:HG22	1:A:467:LYS:HB2	1.79	0.65
1:A:634:ILE:HB	1:A:721:LEU:HB2	1.79	0.65
1:B:425:GLN:HG2	3:B:6139:HOH:O	1.95	0.64
1:A:648:VAL:O	1:A:692:GLU:HA	1.98	0.64
1:B:625:THR:HG21	3:B:6217:HOH:O	1.98	0.64
1:B:100:ARG:HB2	1:B:119:VAL:O	1.98	0.64
1:A:528:VAL:HB	1:A:531:LYS:HG3	1.80	0.64
1:A:559:PHE:HD2	1:B:8:PHE:CE2	2.16	0.63
1:A:663:VAL:HA	1:A:711:SER:HA	1.80	0.63
1:A:605:HIS:HE1	1:A:622:GLN:HE21	1.46	0.63
1:A:659:THR:HG22	1:A:685:PRO:HD3	1.80	0.63
1:B:679:MET:HE1	1:B:681:ARG:HD3	1.81	0.63
1:B:359:ASN:HD21	1:B:570:LYS:HE3	1.64	0.62
1:A:518:VAL:CG1	1:A:619:LEU:HD11	2.29	0.62
1:B:546:ARG:HG3	1:B:546:ARG:NH1	2.14	0.62
1:A:569:LYS:CD	1:A:589:ILE:HD12	2.28	0.62
1:A:629:ILE:HG13	1:A:630:PRO:HD2	1.81	0.62
1:A:335:VAL:HG22	1:A:477:ILE:HD11	1.81	0.62
1:B:516:SER:N	3:B:6294:HOH:O	2.32	0.62
1:B:443:THR:HB	1:B:451:VAL:HG13	1.81	0.62
1:A:637:ARG:HG2	1:A:638:GLY:N	2.15	0.62
1:A:516:SER:O	1:A:517:ASN:HB2	1.99	0.62
1:A:721:LEU:HD23	3:A:6314:HOH:O	1.99	0.62
1:A:268:ALA:HA	1:A:273:GLY:HA3	1.82	0.61
1:A:282:ILE:HG13	1:A:283:TYR:N	2.15	0.61
1:A:569:LYS:HD3	1:A:589:ILE:HD12	1.82	0.61
1:A:623:LYS:HD2	3:A:6156:HOH:O	2.00	0.60
1:B:546:ARG:HH11	1:B:546:ARG:HG3	1.67	0.60
1:B:620:ALA:O	1:B:621:LYS:HG2	2.02	0.60
1:B:424:PHE:HB2	3:B:6348:HOH:O	2.02	0.60
1:A:162:ALA:HB3	1:A:164:TRP:CZ3	2.36	0.59
1:B:437:SER:HB2	1:B:460:ILE:HD13	1.83	0.59
1:B:128:GLY:HA2	1:B:150:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:HB	1:A:451:VAL:CG1	2.31	0.59
1:A:559:PHE:CD2	1:B:8:PHE:HE2	2.21	0.59
1:A:174:ARG:NH2	1:A:179:ASP:OD1	2.37	0.58
1:B:538:THR:HB	1:B:584:LYS:HG2	1.84	0.58
1:B:549:ILE:CG2	1:B:610:ALA:HB1	2.33	0.58
1:A:604:LEU:HB2	1:A:625:THR:HG22	1.84	0.58
1:A:95:ARG:NH1	1:A:96:ARG:NH1	2.52	0.58
1:B:494:LEU:HD22	1:B:494:LEU:O	2.04	0.58
1:B:573:PHE:CE2	1:B:585:GLU:HG3	2.39	0.58
1:B:193:VAL:HG13	1:B:331:PRO:HD3	1.84	0.57
1:A:529:LEU:HD11	1:A:598:LEU:CD1	2.34	0.57
1:A:664:TRP:CD2	1:A:679:MET:HB2	2.39	0.57
1:B:213:PHE:CE1	1:B:474:MET:HB3	2.39	0.57
1:B:648:VAL:O	1:B:692:GLU:HA	2.04	0.57
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.85	0.57
1:A:418:LYS:HD2	1:A:480:THR:O	2.05	0.56
1:A:703:ARG:NE	1:A:703:ARG:HA	2.20	0.56
1:A:313:GLN:H	1:A:316:VAL:HB	1.69	0.56
1:A:682:GLU:CD	1:A:684:ARG:HE	2.08	0.56
1:B:137:ARG:HH11	1:B:137:ARG:CG	2.16	0.56
1:B:385:LEU:HD22	1:B:424:PHE:HB3	1.88	0.56
1:A:95:ARG:HG2	1:A:96:ARG:HD3	1.87	0.56
1:A:287:VAL:CG1	1:A:291:ALA:HB3	2.35	0.56
1:A:354:LEU:CD2	1:A:618:VAL:HG11	2.36	0.56
1:B:553:LEU:HD23	1:B:608:VAL:CG2	2.36	0.56
1:A:355:GLU:HG3	1:A:359:ASN:O	2.04	0.56
1:B:549:ILE:HG22	1:B:550:THR:N	2.21	0.56
1:A:541:ASN:ND2	1:A:579:PRO:HA	2.21	0.56
1:A:559:PHE:HD2	1:B:8:PHE:HE2	1.54	0.56
1:B:31:LEU:HA	1:B:168:GLY:HA3	1.88	0.56
1:A:382:ARG:NH2	1:A:425:GLN:O	2.39	0.56
1:B:715:ARG:HG2	1:B:716:HIS:N	2.21	0.55
1:B:465:VAL:HG21	1:B:474:MET:SD	2.46	0.55
1:B:382:ARG:NH2	1:B:411:PRO:O	2.39	0.54
1:B:553:LEU:O	1:B:570:LYS:HD2	2.08	0.54
1:B:679:MET:HG2	1:B:680:PHE:N	2.22	0.54
1:B:12:ARG:HD2	1:B:16:PRO:HD3	1.90	0.54
1:A:287:VAL:HG12	1:A:288:PRO:O	2.08	0.54
1:A:55:GLU:HG3	1:A:57:TRP:CH2	2.42	0.54
1:B:139:ASP:O	1:B:140:ARG:HB2	2.06	0.54
1:A:559:PHE:CD2	1:B:8:PHE:CE2	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HG2	1:A:164:TRP:CZ3	2.43	0.54
1:A:605:HIS:CE1	1:A:622:GLN:NE2	2.77	0.53
1:B:26:LEU:HD11	1:B:104:VAL:HG11	1.89	0.53
1:B:68:LYS:HE2	1:B:206:LEU:HG	1.91	0.53
1:A:305:SER:O	1:A:306:GLU:HB2	2.06	0.53
1:A:95:ARG:O	1:A:96:ARG:HD2	2.08	0.53
1:A:559:PHE:HB2	1:B:8:PHE:HE2	1.72	0.53
1:B:537:ILE:HD12	1:B:573:PHE:CZ	2.44	0.53
1:B:520:MET:HE2	1:B:621:LYS:HG3	1.90	0.53
1:A:459:HIS:HA	1:A:462:LYS:HE3	1.90	0.53
1:A:541:ASN:HB2	1:A:577:LEU:HD13	1.90	0.53
1:A:678:LYS:HD2	1:A:691:TRP:CD1	2.44	0.53
1:A:335:VAL:O	1:A:374:CYS:HA	2.09	0.52
1:A:281:ASN:HD21	1:A:600:GLU:HG2	1.74	0.52
1:B:664:TRP:O	1:B:709:MET:HA	2.09	0.52
1:A:653:THR:O	1:A:655:PRO:HD3	2.10	0.52
1:B:650:VAL:HG22	1:B:691:TRP:HB3	1.90	0.52
1:B:72:ASN:HD22	1:B:72:ASN:H	1.55	0.52
1:A:425:GLN:HB2	1:A:426:PHE:CD2	2.45	0.52
1:B:549:ILE:HG12	1:B:612:ILE:HG12	1.92	0.52
1:B:541:ASN:O	1:B:580:LEU:HA	2.09	0.51
1:B:284:ALA:HB3	3:B:6521:HOH:O	2.10	0.51
1:B:528:VAL:HB	1:B:531:LYS:HG3	1.93	0.51
1:A:663:VAL:HG13	1:A:709:MET:SD	2.51	0.51
1:A:720:GLU:HG3	3:A:6312:HOH:O	2.09	0.51
1:B:140:ARG:NH1	3:B:6420:HOH:O	2.42	0.51
1:B:553:LEU:O	1:B:570:LYS:HA	2.11	0.51
1:A:331:PRO:HG2	1:A:379:TRP:CB	2.19	0.51
1:A:538:THR:CG2	1:A:582:PHE:CZ	2.93	0.51
1:A:612:ILE:HG22	1:A:613:ASN:N	2.24	0.51
1:B:558:THR:HG22	1:B:564:PRO:HA	1.92	0.51
1:B:662:ASN:N	1:B:662:ASN:HD22	2.07	0.51
1:B:533:PHE:CE1	1:B:589:ILE:HG13	2.46	0.51
1:A:158:ARG:HG2	1:A:174:ARG:CZ	2.41	0.51
1:A:154:VAL:HG21	1:A:184:PHE:CE2	2.46	0.51
1:A:12:ARG:HH22	1:B:406:MET:CE	2.24	0.51
1:A:189:GLU:HA	1:A:194:TYR:CD1	2.46	0.50
1:A:353:PHE:CD2	1:A:364:LEU:HB3	2.46	0.50
1:A:356:GLU:O	1:A:611:ARG:NE	2.44	0.50
1:A:189:GLU:HA	1:A:194:TYR:CG	2.46	0.50
1:B:56:ARG:HD3	3:B:6081:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HG12	3:A:6244:HOH:O	2.11	0.50
1:B:452:VAL:O	1:B:452:VAL:HG13	2.11	0.50
1:A:112:ASN:HB2	3:A:6073:HOH:O	2.11	0.50
1:A:296:VAL:HG21	3:A:6212:HOH:O	2.12	0.49
1:B:136:MET:HB3	1:B:143:ARG:HB3	1.94	0.49
1:A:198:GLU:OE1	1:A:201:ARG:NH1	2.45	0.49
1:B:86:ILE:HD12	1:B:144:LEU:HD11	1.93	0.49
1:A:128:GLY:HA2	1:A:150:PRO:CD	2.42	0.49
1:A:683:ILE:HG12	1:A:689:VAL:HG11	1.94	0.49
1:A:516:SER:N	3:A:6284:HOH:O	2.45	0.49
1:A:209:ILE:HG12	1:A:670:PRO:CG	2.42	0.49
1:A:44:PHE:O	1:A:45:LEU:CB	2.58	0.49
1:A:51:HIS:HB2	1:A:85:GLN:HB3	1.94	0.49
1:B:526:ASN:HB3	3:B:6198:HOH:O	2.13	0.49
1:B:93:ASP:O	1:B:95:ARG:N	2.46	0.49
1:A:552:TYR:O	1:A:608:VAL:HA	2.13	0.49
1:B:331:PRO:HB2	1:B:379:TRP:HB3	1.94	0.49
1:A:568:PHE:HB2	1:A:593:GLU:O	2.13	0.48
1:A:573:PHE:HE1	3:A:6168:HOH:O	1.96	0.48
1:B:454:ASN:ND2	3:B:6060:HOH:O	2.46	0.48
1:B:716:HIS:CE1	3:B:6556:HOH:O	2.66	0.48
1:A:337:ASN:OD1	1:A:461:GLY:HA2	2.13	0.48
1:B:26:LEU:HD12	1:B:160:TYR:CE2	2.48	0.48
1:A:102:GLU:HA	1:A:117:ILE:O	2.13	0.48
1:A:196:ASP:HB2	3:A:6125:HOH:O	2.13	0.48
1:B:137:ARG:HG2	1:B:142:VAL:HG12	1.95	0.48
1:B:537:ILE:HD12	1:B:573:PHE:HZ	1.78	0.48
1:A:313:GLN:OE1	1:A:315:TRP:CH2	2.66	0.48
1:A:68:LYS:HG3	3:A:6049:HOH:O	2.13	0.48
1:B:490:GLU:O	1:B:490:GLU:HG2	2.14	0.48
1:B:551:ALA:HA	1:B:610:ALA:HA	1.96	0.48
1:A:535:LEU:HD23	1:A:536:SER:N	2.29	0.48
1:B:397:SER:HA	1:B:408:ARG:HB3	1.94	0.48
1:A:634:ILE:HD12	1:A:720:GLU:HA	1.96	0.48
1:A:297:ASP:OD1	1:A:297:ASP:N	2.46	0.47
1:B:117:ILE:HG21	1:B:130:TRP:CE2	2.49	0.47
1:A:640:GLN:HG2	1:A:646:MET:SD	2.54	0.47
1:A:81:SER:HA	1:A:146:ILE:O	2.13	0.47
1:B:418:LYS:NZ	1:B:479:ASP:O	2.39	0.47
1:A:339:PHE:HA	1:A:370:TRP:O	2.15	0.47
1:B:213:PHE:CD1	1:B:222:THR:HG22	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:HB3	1:A:706:ILE:HD11	1.96	0.47
1:B:81:SER:HA	1:B:146:ILE:O	2.14	0.47
1:A:652:PHE:O	1:A:688:THR:HA	2.15	0.47
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.79	0.47
1:B:268:ALA:HA	1:B:273:GLY:HA3	1.96	0.47
1:B:402:ASN:HD21	1:B:407:TYR:HB2	1.80	0.46
1:B:633:ILE:HB	1:B:651:GLU:HG3	1.97	0.46
1:B:553:LEU:HD23	1:B:608:VAL:HG22	1.96	0.46
1:A:358:GLY:O	1:A:609:THR:HB	2.15	0.46
1:B:703:ARG:HB2	1:B:723:VAL:HG23	1.97	0.46
1:A:683:ILE:HD11	1:A:689:VAL:HG21	1.98	0.46
1:B:128:GLY:HA2	1:B:150:PRO:CD	2.45	0.46
1:A:163:VAL:N	1:A:170:LEU:O	2.42	0.46
1:A:354:LEU:O	1:A:443:THR:HA	2.15	0.46
1:A:538:THR:HG21	1:A:582:PHE:CZ	2.49	0.46
1:B:705:LEU:O	1:B:720:GLU:HA	2.15	0.46
1:A:153:ILE:HD11	1:A:250:SER:HA	1.98	0.46
1:B:339:PHE:HA	1:B:370:TRP:O	2.16	0.46
1:B:706:ILE:HG21	3:B:6430:HOH:O	2.16	0.46
1:A:8:PHE:CE2	1:B:559:PHE:CD1	3.04	0.46
1:B:559:PHE:HD1	1:B:599:LEU:HD13	1.79	0.46
1:A:128:GLY:HA2	1:A:150:PRO:HD3	1.98	0.46
1:B:660:LEU:O	1:B:682:GLU:HA	2.15	0.46
1:A:667:LEU:HA	1:A:706:ILE:O	2.16	0.45
1:A:418:LYS:HE3	1:A:479:ASP:O	2.16	0.45
1:B:541:ASN:HB2	1:B:577:LEU:HD13	1.98	0.45
1:B:715:ARG:HG2	1:B:716:HIS:H	1.81	0.45
1:A:296:VAL:HB	3:A:6019:HOH:O	2.15	0.45
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.52	0.45
1:B:679:MET:HE2	1:B:679:MET:HB3	1.91	0.45
1:B:297:ASP:N	1:B:297:ASP:OD1	2.49	0.45
1:A:162:ALA:HB3	1:A:164:TRP:HZ3	1.79	0.45
1:A:726:GLN:O	1:A:727:ARG:HB3	2.17	0.45
1:B:18:ASN:HD22	1:B:18:ASN:C	2.21	0.45
1:B:197:ASN:ND2	1:B:200:GLU:OE1	2.42	0.45
1:B:496:THR:O	1:B:499:MET:HG2	2.17	0.45
1:A:355:GLU:O	1:A:611:ARG:NH2	2.49	0.44
1:A:213:PHE:CE1	1:A:474:MET:HB2	2.52	0.44
1:A:520:MET:SD	1:A:608:VAL:HG12	2.57	0.44
1:B:153:ILE:HD11	1:B:250:SER:HA	2.00	0.44
1:B:444:ALA:HA	1:B:450:HIS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ARG:HE	1:A:703:ARG:HA	1.81	0.44
1:A:98:LEU:HG	1:A:164:TRP:HB2	1.99	0.44
1:A:591:ALA:O	1:A:595:MET:HG2	2.17	0.44
1:A:629:ILE:HG13	1:A:717:VAL:HG22	2.00	0.44
1:A:642:VAL:HG21	1:A:700:SER:HB3	1.99	0.44
1:B:213:PHE:CZ	1:B:474:MET:HB3	2.53	0.44
1:A:350:MET:HB3	1:A:350:MET:HE2	1.57	0.44
1:B:568:PHE:CE2	1:B:604:LEU:HG	2.52	0.44
1:B:213:PHE:CE1	1:B:222:THR:HG22	2.51	0.44
1:B:706:ILE:CG2	3:B:6430:HOH:O	2.66	0.44
1:A:91:PRO:HB3	1:A:139:ASP:O	2.18	0.44
1:B:363:LYS:O	1:B:366:LYS:HD3	2.18	0.43
1:B:377:GLU:HB3	1:B:392:TRP:CE3	2.53	0.43
1:B:557:ILE:CD1	1:B:568:PHE:HB3	2.48	0.43
1:A:123:SER:O	1:A:133:LYS:HG3	2.18	0.43
1:A:162:ALA:HB1	1:A:169:VAL:CG1	2.48	0.43
1:B:342:HIS:ND1	1:B:434:GLU:OE2	2.50	0.43
1:B:90:ARG:NH1	1:B:97:ASP:OD2	2.52	0.43
1:A:664:TRP:CE3	1:A:679:MET:HB2	2.53	0.43
1:B:104:VAL:HG12	1:B:116:TYR:HD1	1.84	0.43
1:A:549:ILE:CG2	1:A:550:THR:N	2.78	0.43
1:B:516:SER:N	1:B:617:ASP:OD2	2.52	0.43
1:A:221:LYS:HD2	1:A:221:LYS:HA	1.73	0.43
1:A:697:PRO:HG3	1:A:725:ILE:HD12	2.00	0.43
1:B:557:ILE:HD12	1:B:568:PHE:HD2	1.83	0.43
1:A:681:ARG:HH11	1:A:681:ARG:HG3	1.84	0.42
1:B:44:PHE:O	1:B:45:LEU:CB	2.54	0.42
1:A:51:HIS:HB3	3:A:6432:HOH:O	2.18	0.42
1:B:197:ASN:H	1:B:197:ASN:ND2	2.17	0.42
1:B:519:ASP:HB3	1:B:540:ARG:HD2	2.01	0.42
1:B:518:VAL:HB	1:B:612:ILE:HD11	2.01	0.42
1:A:204:TYR:O	1:A:326:ARG:HG2	2.18	0.42
1:A:490:GLU:HG2	1:A:490:GLU:O	2.19	0.42
1:B:700:SER:HA	1:B:725:ILE:HG22	2.00	0.42
1:B:642:VAL:CG2	1:B:700:SER:HB3	2.49	0.42
1:A:95:ARG:CG	1:A:96:ARG:HH11	2.32	0.42
1:B:650:VAL:HG11	1:B:667:LEU:HD13	2.01	0.42
1:A:636:VAL:HG12	1:A:648:VAL:HG22	2.01	0.42
1:B:353:PHE:CD2	1:B:364:LEU:HB3	2.54	0.42
1:B:557:ILE:HD12	1:B:568:PHE:CD2	2.54	0.42
1:A:589:ILE:N	1:A:589:ILE:HD13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:THR:O	1:A:646:MET:HB3	2.19	0.42
1:B:642:VAL:HG11	1:B:727:ARG:HH22	1.85	0.42
1:A:555:ALA:HA	1:A:605:HIS:O	2.20	0.42
1:A:662:ASN:HB2	1:A:712:ASP:OD1	2.20	0.42
1:B:310:ARG:HA	1:B:311:TYR:HA	1.81	0.42
1:B:565:LYS:HE2	1:B:565:LYS:HB3	1.71	0.42
1:B:641:VAL:HG22	1:B:726:GLN:HB2	2.01	0.42
1:B:237:THR:HG21	1:B:299:LEU:HB3	2.01	0.42
1:A:187:TRP:NE1	1:A:201:ARG:HD2	2.34	0.42
1:A:310:ARG:HA	1:A:311:TYR:HA	1.91	0.42
1:B:440:ILE:HD12	1:B:440:ILE:HG23	1.71	0.42
1:B:549:ILE:CG2	1:B:550:THR:N	2.82	0.42
1:A:678:LYS:HD2	1:A:691:TRP:NE1	2.35	0.41
1:B:187:TRP:CE2	1:B:201:ARG:HD3	2.55	0.41
1:B:472:ASP:OD2	1:B:704:LYS:NZ	2.53	0.41
1:B:556:ASN:HD22	1:B:567:GLU:HA	1.85	0.41
1:B:642:VAL:HG11	1:B:727:ARG:NH2	2.35	0.41
1:A:235:LEU:HA	1:A:327:CYS:SG	2.60	0.41
1:A:45:LEU:HD22	1:A:97:ASP:CG	2.40	0.41
1:A:193:VAL:HG13	1:A:331:PRO:HD3	2.01	0.41
1:A:303:ARG:HG2	3:A:6281:HOH:O	2.21	0.41
1:A:548:THR:HG22	1:A:576:THR:HG23	2.03	0.41
1:B:393:GLN:HB3	1:B:411:PRO:HB2	2.01	0.41
1:A:12:ARG:HH22	1:B:406:MET:HE1	1.86	0.41
1:A:559:PHE:HB2	1:B:8:PHE:CE2	2.54	0.41
1:A:77:ARG:HB3	1:A:185:ASN:HB2	2.02	0.41
1:A:194:TYR:HB3	3:A:6320:HOH:O	2.20	0.41
1:A:269:LYS:O	1:A:270:ASP:HB2	2.21	0.41
1:B:45:LEU:HG	1:B:88:PHE:CD1	2.56	0.41
1:A:313:GLN:OE1	1:A:315:TRP:HH2	2.04	0.40
1:B:611:ARG:HB3	1:B:611:ARG:HE	1.46	0.40
1:A:185:ASN:HD22	1:A:188:CYS:HB2	1.82	0.40
1:A:600:GLU:O	1:A:601:GLN:HB2	2.22	0.40
1:A:636:VAL:HG11	1:A:646:MET:CE	2.52	0.40
1:B:197:ASN:H	1:B:197:ASN:HD22	1.68	0.40
1:B:293:THR:HA	3:B:6430:HOH:O	2.20	0.40
1:B:341:ALA:HB2	1:B:460:ILE:HD13	2.03	0.40
1:B:137:ARG:NH1	1:B:137:ARG:CG	2.82	0.40
1:A:186:PRO:HG2	1:A:205:VAL:HG21	2.03	0.40
1:A:353:PHE:HA	1:A:442:ILE:O	2.22	0.40
1:B:30:GLU:O	1:B:168:GLY:HA3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/731 (95%)	644 (93%)	44 (6%)	7 (1%)	15	11
1	B	701/731 (96%)	662 (94%)	34 (5%)	5 (1%)	22	18
All	All	1396/1462 (96%)	1306 (94%)	78 (6%)	12 (1%)	17	12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	B	45	LEU
1	A	281	ASN
1	A	270	ASP
1	A	196	ASP
1	A	681	ARG
1	A	711	SER
1	A	612	ILE
1	B	34	VAL
1	B	686	ASN
1	B	470	GLY
1	B	94	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	618/644 (96%)	570 (92%)	48 (8%)	12	9
1	B	621/644 (96%)	558 (90%)	63 (10%)	7	4
All	All	1239/1288 (96%)	1128 (91%)	111 (9%)	9	6

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	46	ASN
1	A	47	VAL
1	A	58	ASP
1	A	104	VAL
1	A	112	ASN
1	A	124	GLU
1	A	135	VAL
1	A	195	LEU
1	A	206	LEU
1	A	223	ARG
1	A	271	ASP
1	A	281	ASN
1	A	289	PRO
1	A	301	GLU
1	A	347	ASN
1	A	350	MET
1	A	354	LEU
1	A	364	LEU
1	A	368	SER
1	A	386	PRO
1	A	408	ARG
1	A	415	GLN
1	A	460	ILE
1	A	463	LEU
1	A	465	VAL
1	A	468	GLN
1	A	482	LYS
1	A	488	GLU
1	A	491	ARG
1	A	498	LEU
1	A	516	SER
1	A	523	GLU
1	A	525	GLU
1	A	534	LYS

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Mol	Chain	Res	Type
1	A	553	LEU
1	A	570	LYS
1	A	572	THR
1	A	587	VAL
1	A	597	GLN
1	A	604	LEU
1	A	616	ARG
1	A	625	THR
1	A	629	ILE
1	A	637	ARG
1	A	661	ARG
1	A	681	ARG
1	A	721	LEU
1	B	12	ARG
1	B	14	VAL
1	B	18	ASN
1	B	20	ASN
1	B	42	GLN
1	B	46	ASN
1	B	72	ASN
1	B	76	VAL
1	B	98	LEU
1	B	112	ASN
1	B	137	ARG
1	B	138	GLU
1	B	140	ARG
1	B	147	GLN
1	B	164	TRP
1	B	167	TYR
1	B	169	VAL
1	B	172	THR
1	B	174	ARG
1	B	195	LEU
1	B	206	LEU
1	B	223	ARG
1	B	235	LEU
1	B	239	LEU
1	B	304	SER
1	B	340	SER
1	B	359	ASN
1	B	408	ARG
1	B	451	VAL

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Mol	Chain	Res	Type
1	B	455	VAL
1	B	463	LEU
1	B	465	VAL
1	B	468	GLN
1	B	482	LYS
1	B	484	GLN
1	B	488	GLU
1	B	489	GLU
1	B	494	LEU
1	B	498	LEU
1	B	507	ASN
1	B	519	ASP
1	B	520	MET
1	B	531	LYS
1	B	538	THR
1	B	540	ARG
1	B	546	ARG
1	B	557	ILE
1	B	559	PHE
1	B	571	GLU
1	B	574	ASP
1	B	578	GLU
1	B	588	LEU
1	B	589	ILE
1	B	604	LEU
1	B	611	ARG
1	B	625	THR
1	B	626	VAL
1	B	637	ARG
1	B	639	THR
1	B	656	LEU
1	B	704	LYS
1	B	721	LEU
1	B	727	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	112	ASN
1	A	267	ASN
1	A	281	ASN

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	526	ASN
1	A	597	GLN
1	A	605	HIS
1	A	622	GLN
1	B	18	ASN
1	B	72	ASN
1	B	112	ASN
1	B	359	ASN
1	B	450	HIS
1	B	468	GLN
1	B	484	GLN
1	B	545	ASN
1	B	556	ASN
1	B	613	ASN
1	B	662	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.